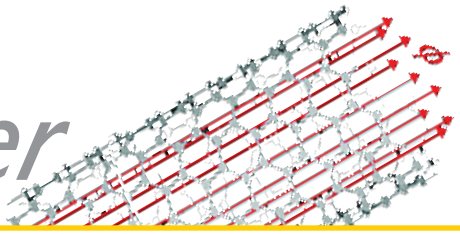
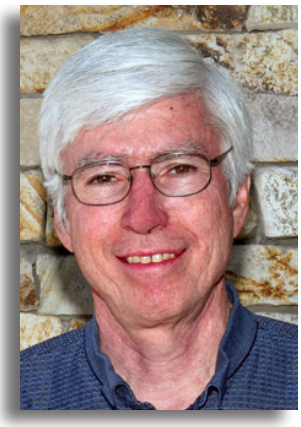
MPA materials matter

March 2008

Newsletter of the Materials Physics and Applications Division





Tom Picraux is seeking suggestions for technical symposia for the 2009 AAAS annual meeting and for candidates for fellowship (picraux@lanl.gov).

Picraux chair-elect of AAAS industrial science and technology section

Tom Picraux, Center for Integrated Nanotechnologies (CINT) chief scientist, was recently elected incoming chairman of the AAAS (American Association for the Advancement of Science) section on industrial science and technology.

Duties of the section include organizing and sponsoring technical symposia and topical lectures at the AAAS annual meetings and encouraging nominations for AAAS fellowship. The industrial S & T section is a rapidly growing section of AAAS with more than 2,800 affiliated members.

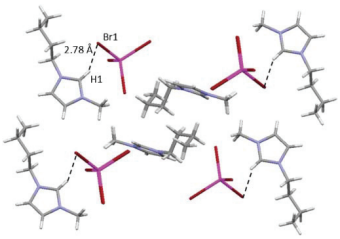
Picraux, who began his term as chair-elect in February, is seeking suggestions for technical symposia for the 2009 AAAS annual meeting and for candidates for fellowship (picraux@lanl.gov).

Picraux joined CINT in 2005 from Arizona State University where he was professor and executive director of materials research. He is a fellow of the American Physical Society and the AAAS. Picraux, who earned his PhD in engineering science and physics from California Institute of Technology, is a recipient of the Department of Energy's E.O. Lawrence Award for his work in materials research.

INSIDE this issue

MPA article on ionic liquids one of 10 most accessed in online *Chemical Communications*

An article on the structure and magnetic behavior of transition metal based ionic liquids by MPA-MC researchers and collaborators was one of the top 10 accessed articles on the web from the online version of *Chemical Communications*. In January alone the article received 1,515 accesses, placing it within the top ten.



Structural view of one of the transition metal-based paramagnetic anions.

In the article, the researchers report on a series of ionic liquids containing different paramagnetic anions that they prepared. Although the ionic liquids are simply paramagnetic, they respond strongly to an applied magnetic field. The tetraalkylphosphonium-based ionic liquid's behavior is somewhat anomalous. The extreme hydrophobicity of the phosphonium ionic liquids allows droplets of them to be manipulated by an external magnet through a matrix of water. These materials have potential applications for magnetic and electrochromic switching as well as novel magnetic transport.

"Structure and Magnetic Behavior of Transition Metal Based Ionic Liquids," by Rico Del Sesto, Mark McCleskey, Anthony Burrell, and Brian Scott, all MPA-MC; Joe Thompson, MPA-10; G. A. Baker, Oak Ridge National Laboratory; and J. Wilkes and P. Williams, U.S. Air Force Academy, appears in *Chem. Commun.*, **447** (2008). The Laboratory-Directed Research and Development program supported the Los Alamos portion of the work.

Technical contact: Rico Del Sesto, ricod@lanl.gov

Now that's MPA!

Express your vision in icon contest

MPA Division is holding a contest to create a graphical icon that represents the best of our Division's diversity, vitality, and expertise. Use your creativity and share your concept of how you see materials physics and applications at Los Alamos. The MPA Council will review submissions and determine which will be the basis for the MPA icon, to be used in a variety of Division products. The creator of the winning entry will receive a gift certificate.

Guidelines

- Deadline for entries to kkippen@lanl.gov is April 30
- Send your entry in its original and .pdf formats.
- When creating, keep in mind the icon will be used in a variety of formats and sizes.
- Have technical content ADC reviewed before submitting.

From Alex's desk

Materials Physics and Applications: Building our future

As part of building our future as an institution we must plan what we will do and how we will accomplish the endeavors we set for ourselves. In doing so, it is of paramount importance to set realistic expectations and to acquire the needed support. As I stated in a couple recent group and center meetings I attended, planning our future is exactly what the individual performance objective (IPO) process should be about. Following the EPS Directorate-wide organizational objectives set forward by Susan Seestrom, I have composed a set of integrated MPA organizational objectives that have been distributed to your group and center leaders. Starting this year, our IPOs will have a behavior-based component. I encourage you to become engaged in the process. Please begin to discuss your goals and work with your local leadership to define what we can do to help you succeed.

MPA staff in the news: MPA-CINT Chief Scientist Tom Picraux was recently elected a fellow of the Materials Research Society. His citation was for "leadership in the application of ion channeling and ion beam materials modification to materials research, and in the advancement of materials science through research management and professional society service." Tom's previous pioneering work was in ion beam modification and analysis of electronic materials. His recent work is on the vapor-liquid-solid growth of nanowires.

MPA-STC Deputy Center Leader Ken Marken has been appointed to the editorial advisory board for the Institute of Physics journal *Superconductor Science and Technology*. Founded in 1988, *SuST* is the journal for all aspects of superconductivity with the highest impact factor (1.440) of all journals specializing in this field. Ken's appointment runs through December 2009.

Experimental work performed at the magnet laboratory by MPA-NHMFL's Susan Cox, John Singleton and MST-6's Jason Lashley in collaboration with staff from Cambridge, and Edinburgh, has been selected one of the top 10 papers in the *Journal of Physics: Condensed Matter (JPCM)*. In making the selection, David Ferry, the journal's editor-in chief, said, "The choice is difficult because *JPCM* has succeeded in attracting many excellent and innovative authors. Our very fair but rigorous referees have ensured a consistently high standard of papers in the journal. Many more papers were singled out with the support of referees (identifying work of the very highest importance), of readers (through high numbers of full-text downloads), and of our board members (through recommending articles they found especially valuable." The work, "Is the stripe phase a charge density wave?" (S. Cox, J. C. Lashley, E. Rosten, J. Singleton, A. J. Williams and P. B. Littlewood, appears in *J. Phys.: Condens. Matter* **19** (192201) (2007). By measuring heat capacity on three manganite materials, the team established that the transition at which the stripe phase appears in manganites is second order and is accurately modeled as a Peierls transition. It is important to notice that this result adds to the growing body of evidence that the stripe and ferromagnetic phases are much more similar than previously thought and indicates that the colossal magnetoresistance present in manganites is driven by the delicate balance between the ferromagnetic and stripe phase.

Fitting of transition peaks for three compounds to a model of a Peierls transition in a system with impurities (a linear background was removed). Points are data and the solid line is the fit of the model to the data. New measurements point to the charge-density-wave nature of the stripe phase in manganites

MPA-11 welcomes Bettina Reardon to the fuel cell team as a chemical technician for the hydrogen fuel quality and sensor development projects. Bettina began her chemical technician career at Los Alamos in 1994 in MPA-STC synthesizing high temperature superconductor ceramic composites. From there she worked with a nuclear material research team at TA-55 applying solid-liquid separations techniques to aqueous chloride processing. In 1997 she transferred to the Polymers and Coatings Group (MST-7) where she performed a variety of characterization analysis.

MPA-NHMFL welcomes Rhonda Carter as the new group office administrator. Rhonda comes to the NHMFL from P-24 and has more than 20 years of experience at the Laboratory, having worked at different offices. She has extensive experience with the Laboratory's foreign national program and visitor programs, travel systems, Data

"Desk, "continued on page 3

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EPS Communications,
at 606-1822, or kkippen@lanl.gov.

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To read past issues see
www.lanl.gov/orgs/mpa/materialsmatter.shtml

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Findings to appear in Physical Review E

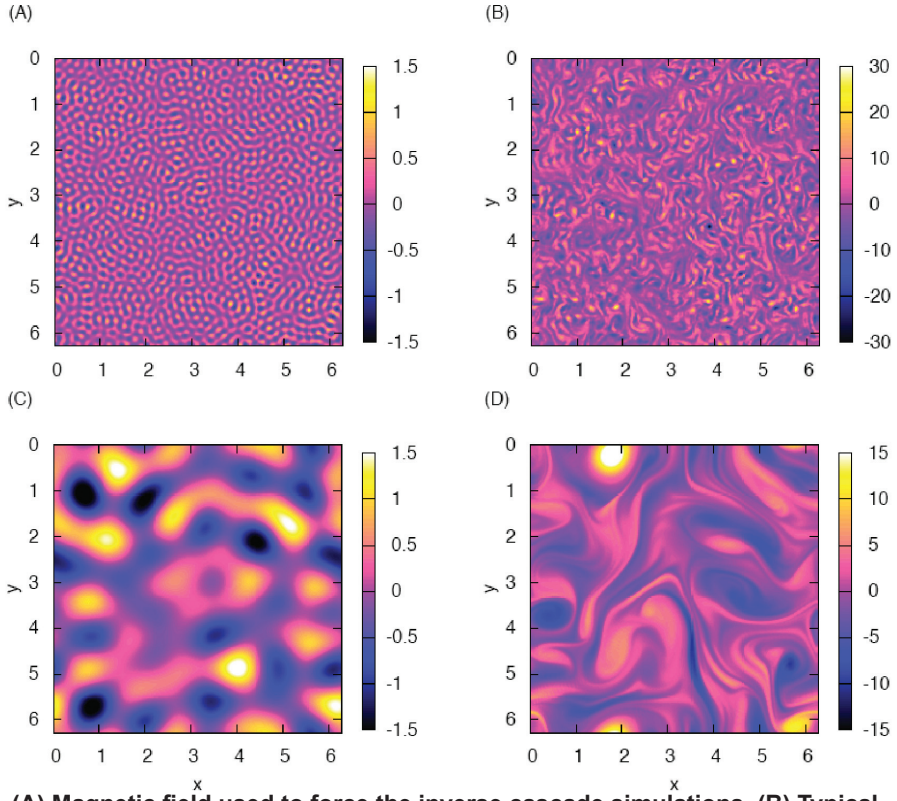
Modeling power fluctuations in turbulent flows

Power fluctuations of a Brownian particle follow a Gaussian distribution owing to random energetic kicks received from the environment. In contrast, a particle in a turbulent flow is subject to power fluctuations that arrive in correlated intermittent bursts.

In *Physical Review E*, in press, Mahesh Bandi, MPA-10, and Colm Connaughton, T-13, study the statistics of power for such a particle in simulated two-dimensional turbulence, an idealization of atmospheric turbulence. Their study has implications for engineered systems as it relates to the power required to overcome turbulent drag to sustain the rotation of a fan or turbine at a given speed in a turbulent flow. From a more fundamental standpoint, their studies may lead to a better understanding of nonequilibrium dissipative phenomena, of which turbulence is a prime example.

In this study, the power ($p = f \cdot v$) (force (f) and velocity (v) both having Gaussian distributions but correlated with each other) exhibits a distribution with wide asymmetric non-Gaussian tails centered at $p = 0$ with a logarithmically divergent singularity. The power distribution is accurately modeled by knowing only three variables, the standard deviations of f and v and their instantaneous correlation coefficient. Though derived specifically for two-dimensional turbulence (see figure), this model is generally applicable to any nonequilibrium process where the quantity of interest is a product of two normally distributed variables that are correlated with each other, e.g. heat flux in thermal convection or transport of matter on an ocean's surface. This work is a collaboration between postdoctoral researchers Bandi and Connaughton, both holding joint appointments with the Center for Nonlinear Studies (T-CNLS). The CNLS program on multi-scale modeling of strongly interacting systems funded the work.

Technical contact: Mahesh Bandi, mbandi@lanl.gov



(A) Magnetic field used to force the inverse cascade simulations. (B) Typical vorticity snapshot from the inverse cascade. (C) Magnetic field used to force the direct cascade simulation. (D) Typical vorticity snapshot from the direct cascade.

"Desk" Continued from page 2

Warehouse, and the time and effort system.

Finally, please keep engaging with MPA's WSST members. Any team member would be happy discussing and working with you on any safety issues. MPA- WSST members are Chris Sheehan (chair), MPA-STC; Eric Bauer, MPA-10; Roger Lujan, MPA-11; Clay Macomber, MPA-MC; Chuck Mielke, MPA-NHMFL; Darrell Roybal, MPA-NHMFL, and Darrick Williams, MPA-CINT. For more information about MPA-WSST, please visit int.lanl.gov/orgs/mpa/mpa_wsst.

Interim MPA Division Leader Alex H. Lacerda

Celebrating service

Heads UP, MPA!

MPA WSST, working for you

The MPA Worker Safety and Security Team (WSST) has been working since September on issues raised by MPA employees. You'll be seeing us here in Heads Up, MPA! with a monthly summary of our minutes and things we think you should know. If you have any safety or security concerns (urgent issues should go to your safety and security representatives first) or related policy issues that don't make sense and are getting in the way of your work, let us know.

To date, issues the WSST has worked on include the following:

- Card readers at NHMFL
- Exhibit F and G
- Swagelok training
- Facility/programmatic equipment maintenance
- Gas plant procedures related to ChemLog
- X-ray generating device log book requirements
- FOD and ES&H contacts
- Glovebox requirements and fire extinguisher training.

Some of these issues were worked on for months (and are still ongoing), due in part to trying to determine who generated a policy and why. Many times we quickly came to the conclusion that a Laboratory-wide policy was the problem and was not specific to MPA.

See our Web site, int.lanl.gov/orgs/mpa/mpa_wsst/, and view our action log and minutes for more details on the above items.

Gas cylinder notice

If you are a gas purchaser or handle gas cylinders directly, you should have received an email recently from your group's MPA WSST member. To summarize:

- The gas plant has a new website that we helped them correct, int.lanl.gov/orgs/os/pt/gas/.
- It is your responsibility to ensure your ChemLog records are up to date even though the gas plant notices state that it will take care of ChemLog "disposal."
- ChemLog stickers are not to be removed from cylinders. Instead, keep a written list of the barcode numbers from cylinders you return to the gas plant in case of inventory discrepancies

MPA WSST Spot Awards

Your MPA WSST has been given Spot Awards from MPA-DO to recognize MPA employees who bring the team important issues or who set a good example for exceptional safety and security practices. Talk to your group's MPA WSST member or send us an email at mpawsst@lanl.gov if you have issues or suggestions.

MPA WSST members

Your MPA contacts are:
Chris Sheehan (chair), MPA-STC, *sheehan@lanl.gov*
Eric Bauer, MPA-10, *edbauer@lanl.gov*
Roger Lujan, MPA-11, *rwlujan@lanl.gov*
Clay Macomber, MPA-MC, *macomber@lanl.gov*
Chuck Mielke, MPA-NHMFL *cmielke@lanl.gov*
Darrell Roybal, MPA-NHMFL, *daroybal@lanl.gov*
Darrick Williams, MPA-CINT, *darrick@lanl.gov*

Heads UP, MPA! reports on environment, safety, and health, security, and facility-related news and information.

Tracking single quantum dots in three dimensions

Researchers working at the Center for Integrated Nanotechnologies (MPA-CINT's Guillaume Lessard, Peter Goodwin, and Jim Werner) have recently developed instrumentation that can follow individual quantum dots moving through three-dimensional space at rates faster than many intracellular transport processes.

These experiments show three-dimensional tracking of quantum dots in glycerol/water mixtures using a home-built confocal microscope that uses active feedback to re-center the quantum dot back to the center of the optical probe volume 200 times/second.

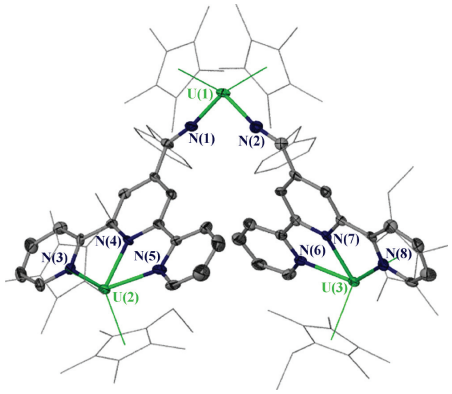
The method and instrument will be extremely useful for studying intracellular transport, for performing single molecule spectroscopy measurements in live cells, and for studying soft materials that possess heterogeneity and anisotropy over multiple length scales.

As single element detectors (and not CCD cameras) are employed the system can perform time-resolved spectroscopy on the molecules being tracked. In addition to following individual quantum dots this system has the sensitivity needed to follow the three-dimensional motion of individual green fluorescent proteins and individual organic fluorophores.

The work, "Three-dimensional tracking of individual quantum dots," appears in *Applied Physics Letters* **91**, 224106 (2007) and was supported by the Los Alamos Laboratory Directed Research and Development program, the Los Alamos Technology Transfer maturation fund, and the National Nanotechnology Enterprise Development Center. The team (PI: Werner) has recently received an exploratory grant (R21AI077072, $519,767) from the National Institutes of Health to demonstrate the microscope can be used to study intracellular transport.

MPA researchers study uranium multimetallic complexes

Recent studies have shown that multimetallic molecular systems may serve as models for understanding electronic structures in complex actinide materials, wherein 5f/6d electrons can span the continuum from core-like and non-bonding to delocalized and involved in bonding with appreciable covalent character. Therefore researchers synthesized and studied two rare multimetallic complexes of actinides in a low valent state, which were proven to be pivotal in gaining a further understanding of the electronic and magnetic coupling between mixed lanthanide/actinide ligand bridge complexes. The ligand synthesis capability in Bioscience Division (B-8) provided a variety of molecular designer scaffolds, which help to control the bonding structure and electronic state of mixed-valent homo- and hetero-trimetallic actinide complexes. A manuscript "Mixed-Valency in Uranium Multimetallic Complexes" by Eric J. Schelter, MPA-10; Rulian Wu, B-8; Brian L. Scott, MPA-MC; Joe D. Thompson, MPA-10; David E. Morris, C-PCS; and Jaqueline L. Kiplinger, MPA-10, has been accepted for publication as a communication in *Angewandte Chemie*. The research was supported through the Los Alamos National Laboratory Frederick Reines's and Director's Postdoctoral Fellowships, the Laboratory-Directed Research and Development program, and the Division of Sciences, DOE Office of Basic Energy Sciences, Heavy Element Chemistry program.



X-ray crystal structure of a uranium multimetallic complex.

First observation of coupling between an optical phonon and the Kondo effect

For more than forty years, there has been significant interest in the screening of local moments by conduction electrons, termed the Kondo effect. Since its discovery, the Kondo effect has produced a number of surprising results, including heavy Fermion compounds where the carriers are extremely massive. Kondo later suggested that the conduction electrons could also screen the motion of atoms. It has since been proposed that coupling between lattice vibrations and the Kondo effect could manifest new material properties, such as unconventional superconductivity and a break down of the Fermi liquid theory, a cornerstone of modern condensed matter. Furthermore, such coupling has produced new effects in other systems, such as colossal magneto-resistance and multi-ferroic behavior in transition metal oxides. However, despite extensive work on the Kondo lattices, there have been no observations of coupling between the Kondo effect and an optical phonon mode, in part because it has been unclear how to detect such a coupling.

The 14-1-11 family of compounds is a particular interesting and promising series of compounds to explore since the lattice plays an important role. Specifically, various properties can be altered through iso-electronic substitutions. The 14-1-11 compounds exhibit numerous ground-states, including magnetic order, metallic or semiconducting transport, and HF behavior. Of particular interest is $Yb_{14}MnSb_{11}$, which is metallic and exhibits ferromagnetic order of the Mn d4 local moment below a Curie temperature of 53 K. A study of its optical conductivity suggested that the Mn d-shell has a fifth electron that is screened by the Kondo effect. It was argued that the coexistence of ferromagnetism and heavy Fermion behavior occurs via a distortion of the $MnSb_4$ tetrahedron motivating a search for Kondo-lattice coupling in $Yb_{14}MnSb_{11}$.

MPA-CINT researchers recently demonstrated Kondo-phonon coupling in $Yb_{14}MnSb_{11}$ by simultaneously monitoring the electronic structure and lattice vibrations via ultra-fast optical experiments. Specifically, well-established signatures of the development of a heavy liquid state are seen in the ultra-fast optical response of $Yb_{14}MnSb_{11}$, namely an anomalous increase in the amplitude and relaxation time. From this data, the researchers could quantify, at various temperatures, the number of electrons in the system that had become heavy. Furthermore, their optical pulses excited lattice vibrations that they could then detect, such that the frequency of the vibration as a function of temperature could also be determined.

Interestingly, at low temperatures the phonon frequency was significantly decreased, an effect that could be described quantitatively via the development of the heavy Fermion state. This work, which will appear in *Physical Review Letters*, therefore provides a blueprint for future examination of Kondo-phonon coupling in other heavy Fermion compounds.

Researchers include Ken Burch, Toni Taylor, Elbert Chia, Diyar Talbayev, Rick Averitt, MPA-CINT; and Brian Sales and David Mandrus, Oak Ridge National Laboratory.

The work was funded by the Laboratory-Directed Research and Development program.